TABLE IV

DEBYE–SCHERRER PATTERN OF NaCl-TYPE SnP AND CALCULATED INTENSITIES FOR NaCl-TYPE AND SPHALERITE-TYPE SnP (λ(Cu Kα) 1.54178 Å, $a = 5.535 \pm 0.001$ Å)[a]

I/Io obs.	h	k	l	d (obs.)	d (calc.)	I calc. (NaCl type)	I calc. (Sphalerite type)
90	1	1	1	3.2177	3.1955	84	159
100	2	0	0	2.7748	2.7674	123	44
65	2	2	0	1.9599	1.9568	89	89
50	3	1	1	1.6703	1.6688	38	68
45	2	2	2	1.5998	1.5977	31	11
20	4	0	0	1.3847	1.3837	14	14
15	3	3	1	1.2704	1.2693	15	27
40	4	2	0	1.2377	1.2370	38	14
25	4	2	2	1.1300*	1.1298	29	32
10	5	1	1	1.0049*	1.0051	9	16
15	4	4	0	.9784*	.9784	11	11
15	5	3	1	.9357*	.9359	16	29
20	6	0	0	.9225*	.9224	5	2
20	6	2	0	.8751*	.8751	24	24
5	5	3	3	.8441*	.8440	10	17
15	6	2	2	.8343*	.8344	29	11
						R = 16.4%	R = 51.0%

[a] Asterisks signify λ(Cu $K\alpha_1$) 1.54051 Å.

Discussion

The formation of two new high-pressure forms of SnP has been shown. It is unclear which phase is the more stable at 65 kbars and why the two phases are intimately mixed. X-Ray diffraction at high pressure may perhaps resolve the phase relationships. The cubic phase should be the high-pressure phase since the density is greater. The calculated density of the cubic phase is 5.860 g/cm³ while the calculated density of the tetragonal phase is 5.68 g/cm³. The cubic form may be present at high pressure and upon quenching may revert partially to the tetragonal phase. The transformation from tetragonal to cubic upon heating at atmospheric pressure is interesting since it involves a transformation from a less dense to a more dense phase.

The crystal structure of the tetragonal phase has been shown to be similar to that of high-pressure GeP and GeAs.[9] The structure (Figure 1) is related to the NaCl type by a small shifting of atoms. If the diagonal on the basal plane equaled the c axis and $z = 0.5$, the structure would be NaCl type. The atoms are in a distorted octahedral arrangement having one short bond, four slightly longer equal bonds, and one long bond. The shift to the cubic structure involves a regularization of the octahedron. The crystal structure of SnAs[8] is known to be NaCl type and implies that as the elements become more metallic the NaCl-type structure is favored. Both forms of SnP are metallic conductors. This may be because the compounds have one extra electron for conduction. The tetragonal forms of GeP and GeAs showed superconductivity;[9] however, only the cubic SnP was seen to be superconducting above 1.25° K.

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